TITLE: COMPUTATIONAL AND EXPERIMENTAL MODELING OF SLURRY-BUBBLE COLUMN REACTORS

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ABSTRACT

OBJECTIVE

This project is a collaborative effort between two universities (Akron University and Illinois Institute of Technology) and two industries (UOP and Energy International). The overall objective of this research is to develop predictive hydrodynamic models for gas-liquid-solid catalyst reactors using computational fluid dynamics (CFD) techniques. The work plan involves a combination of computational, experimental and theoretical studies with a feedback mechanism to correct model deficiencies. The tasks involve : 1- Development of a CFD code for slurry bubble column reactors. 2- Optimization. 3- Comparison to reactor data. 4- Development of a three dimensional transient CFD code. 5- Measurement of particle turbulent properties. 6- a) Measurement of thermal conductivity of particles in the IIT two story riser. b) Measurements of evaporation rates of liquid nitrogen in the IIT riser.

ACCOMPLISHMENTS TO DATE

Our paper describing the basic approach using kinetic theory to predict the turbulence of catalyst particles in a slurry bubble column reactor, has been published in a refereed journal (Wu and Gidaspow, 2000). The computed slurry height, gas hold up and rate of methanol production agreed with the Department of Energy La Porte pilot plant reactor data.

We have invented an alternate technique for computing turbulence in a slurry bubble column. It involves direct numerical simulation of the equations of motion with the measured particular viscosity as an input. We have computed the flow profiles, particle concentration profiles and Reynolds stresses for an IIT slurry bubble column. The computed time averaged particle velocities and concentrations agree with PIV measurements of velocities and concentrations, obtained using a combination of gamma-ray and X-ray densitometers, in a slurry bubble column, operated in the bubbly-coalesced fluidization regime with continuos flow of water. Both the experiment and the simulation show a down-flow of particles in the

center of the column and up-flow near the walls and nearly uniform particle concentration. The computations were done using our previous two dimensional three phase code and a newly developed three dimensional version. This work was reported in the Ph.D. thesis by Diana Matonis (IIT, 2000) and in a paper submitted for publication and presentation in ICMF 2001.

Measurements of thermal conductivity of catalyst particles in the IIT riser were completed. The IIT riser was redesigned to eliminate asymmetries, similarly to the Sandia National Laboratory riser, sponsored by the Multiphase Fluid Dynamics Research Consortium. Our CCD camera system was used to measure Reynolds stresses and granular temperature for 450 μm glass beads. The granular temperature when computed, following the gravity wave, shows a maximum in the center, in agreement with conventional theory of granular flow. Numerical simulation of the riser is in progress.

In an attempt to optimize the system, flow patterns for the production of methanol in slurry bubble columns were investigated by rearranging the location of the heat exchangers in the La Porte pilot plant.

SIGNICANCE TO FOSSIL ENERGY PROGRAMS

Indirect liquefaction is a two stage process that employs a gasification technology to first produce synthesis gases from coal. The synthesis gases are then converted to various hydrocarbon products and oxygenates in a slurry bubble column reactor in the presence of catalyst and solvent. The indirect liquefaction technology is being developed by DOE/Air Products at the La Porte Alternative Fuels Development Unit, Exxon, Shell, Sasol and Energy International Corporation, a subsidiary of Williams Field Services.

ARTICLES AND PRESENTATIONS

Journal Articles

- Wu Y. and D. Gidaspow, "Hydrodynamic simulation of methanol synthesis in gas-liquid slurry bubble column reactors", Chem. Eng. Sci., 55, 573-587, 2000.
- Matonis D., D. Gidaspow and M. Bahary, "CFD Simulation of Flow and Turbulence in a Slurry Bubble Column Reactor", submitted to AIChE J., to be presented in ICMF 2001, New Orleans, Louisiana, May 2001.

Conference Presentations

- Gidaspow D., "Fluidized Bed Hydrodynamics and Direct Contact Heat Transfer using Kinetic Theory", Festschrift session, 33rd National Heat Transfer Conference, Albuquerque, New Mexico, Aug. 15-17, 1999.
- Gidaspow D., Wu Y. and R. Mostofi, "Turbulence of Particles in a CFB and Slurry Bubble Columns using Kinetic Theory", Fluidization and Fluid-Particle Systems Preprint Volume, AIChE, pp. 261-266, AIChE Annual meeting, Dallas, Texas, Oct. 31-Nov. 5, 1999.
- Gidaspow D., Mostofi R., Tartan M., Vijayaraghavan K., Sharma B., Matonis D. and Y.S. Shin, "Computation and Measurement of Structure and Turbulence in Risers and Bubbling Beds", Multiphase Fluid Dynamics Research Consortium Annual Meeting, Albuquerque, New Mexico, Apr. 12, 2000.
- Gamwo I., Halow J.S., Gidaspow D., Mostofi R. and Matonis D., "CFD models for slurry bubble column reactors", 5 th International Conference on Gas-Liquid and Gas-Liquid-Solid Reaction Engineering World Congress, Melbourne, Australia, September 2001.